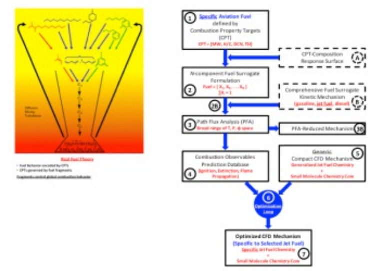
Compact Kinetic Mechanisms for Petroleum-Derived and Alternative Aviation Fuels, Phase II Project

SBIR/STTR Programs | Space Technology Mission Directorate (STMD)

ABSTRACT

To be useful for computational combustor design and analysis using tools like the National Combustion Code (NCC), low-dimensional chemical kinetic mechanisms for modeling of real fuel combustion chemistry must be sufficiently compact so that they can be utilized in multi-dimensional, multi-physics, reacting computational fluid dynamics (CFD) simulations. Despite advances in CFD-appropriate kinetic mechanism reduction for kerosene-range fuels, significant combustion property variation among current and prospective certified fuels remains a challenge for meaningful CFD-advised design of high pressure, low-emissions combustors. The proposed project will leverage Princeton's ongoing work in aviation fuel surrogate formulation and modeling as well as kinetic mechanism development for emissions and high pressure combustion to produce and demonstrate a meta-model framework for automated generation of fuel-flexible compact chemical kinetic mechanisms appropriate for 3-D combustion CFD codes. During Phase I, Compact Mechanisms for both an alternative, natural-gas derived synthetic kerosene and a conventional petro-derived Jet A kerosene have been developed and demonstrated. Results indicated that, over a very broad range of pressures, temperatures, equivalence ratios, and characteristic times, these Compact Mechanisms well reproduce predictions of global combustion behaviors (ignition, extinction, heat release rate, pollutant mole fractions) relative to predictions of significantly larger target chemical kinetic mechanisms. Technical objectives for Phase II R&D include development of a stand-alone software application for generation of tailor-made, fuel-specific Compact Mechanisms, and demonstration of Compact Mechanism performance in computation-intensive CFD applications. Achievement of these objectives together will advance the current state of this R&D program to TRL 5.



Compact Kinetic Mechanisms for Petroleum-Derived and Alternative Aviation Fuels

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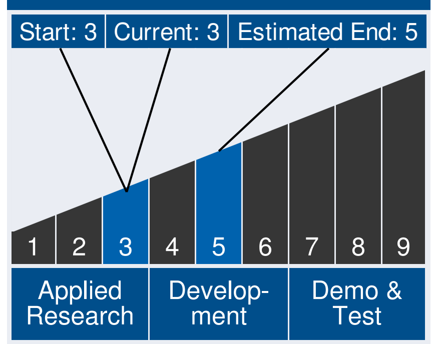
Technology Maturity



Management Team

Program Executives:

- Joseph Grant
- Laguduva Kubendran

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ANTICIPATED BENEFITS

To NASA funded missions:

Potential NASA Commercial Applications: The Technical Objectives presented in this Phase I proposal directly address a topic in the NASA SBIR solicitation for low emissions/clean power aircraft combustors. The "compact" low-dimensional chemical kinetic mechanisms proposed for modeling of real aviation fuel combustion chemistry will support physics-based CFD development of next-generation engines such as those employing lean direct injection (LDI) technology. Reacting flow simulation platforms like NASA's National Combustion Code (NCC), as well as ANSYS, KIVA, and OpenFOAM, require mechanisms sufficiently compact so as to be tractable for multi-dimensional, multi-physics, CFD simulations, but which also preserve the predictive fidelity of more detailed kinetic mechanisms. Importantly, the present framework permits the consideration of a variety of real fuels, including alternative fuels derived from a variety of non-petroleum resources. Evaluation of such alternative fuels is among the major NASA research thrusts under the general topic of propulsion.

To the commercial space industry:

Potential Non-NASA Commercial Applications: The commercial product foreseen from this SBIR program is a stand-alone, novice-friendly real fuel kinetic mechanism generator software package that can interface with commercially-available computational fluid dynamics (CFD) codes. Accordingly, potential customers may include the companies supplying ANSYS, CFD-ACE+, or COMSOL, as well as industrial users with proprietary in-house codes. Application of compact real fuel kinetic models has broad appeal to automotive, aerospace, and marine propulsion industries, both for civilian and DoD applications.

Management Team *(cont.)*

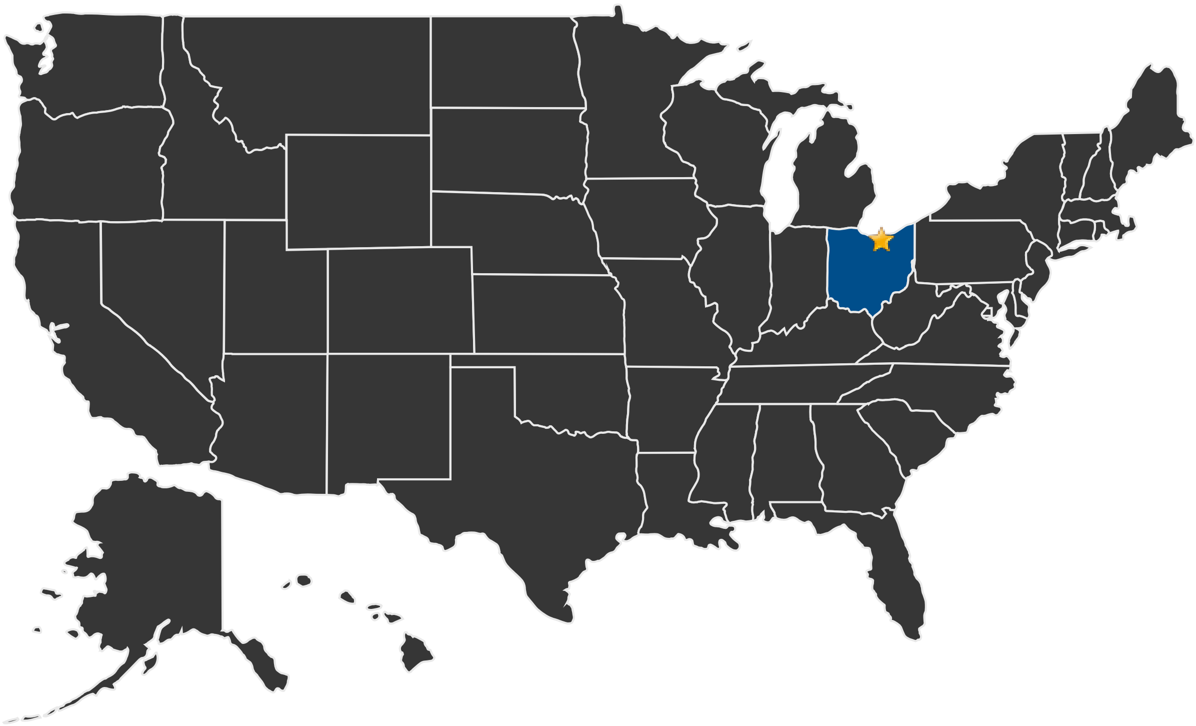
Program Manager:
- Carlos Torrez

Principal Investigator:
- Sivaram Gogineni

Technology Areas

Secondary Technology Area:
In-Space Propulsion Technologies (TA 2)
└ Chemical Propulsion (TA 2.1)
  └ Liquid Storable (TA 2.1.1)

U.S. WORK LOCATIONS AND KEY PARTNERS



U.S. States With Work

Lead Center:
Glenn Research Center

Other Organizations Performing Work:

- Spectral Energies, LLC (Dayton, OH)

PROJECT LIBRARY

Presentations

- Briefing Chart
  - (http://techport.nasa.gov:80/file/17840)

DETAILS FOR TECHNOLOGY 1

Technology Title

Compact Kinetic Mechanisms for Petroleum-Derived and Alternative Aviation Fuels